

A new kinetic equation for dense gases

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Abstract. Alexander, Garcia and Alder [1] introduced the Consistent Boltzmann Algorithm (CBA) as a simple variant of Direct Simulation Monte Carlo (DSMC) for dense gases. In CBA, collisions alter both the positions and velocities of the particles. In the present work the limiting kinetic equation for CBA is derived; the formulation is similar to the proof that the Boltzmann equation is the limiting kinetic equation for DSMC [11]. The relation between this new kinetic equation and the Enskog equation is outlined.

INTRODUCTION

Direct Simulation Monte Carlo (DSMC) is presently the most widely used numerical algorithm in kinetic theory [3]. The limiting kinetic equation for DSMC is the nonlinear Boltzmann equation [11] so its application is restricted to dilute gases. In DSMC, particle pairs are randomly chosen to collide according to the collision probability for the interparticle potential. For example, for the hard sphere potential this probability is proportional to the particles' relative speed. The post-collision velocities are determined by randomly selecting the collision angles and the number of collisions on each time step is computed from the local collision frequency. Note that in DSMC particles can be chosen to collide even if their actual trajectories do *not* overlap.

Recently, the Consistent Boltzmann Algorithm (CBA) was introduced as a simple variant of DSMC for dense gases [1]. Although CBA can be generalized to any equation of state [2] here we will only consider the hard sphere gas with particle diameter σ . In CBA the collision process is as in DSMC with two additions. First, when a pair collides the unit apse vector, e , that is, the unit vector parallel to the line connecting the centers at impact, is computed from the pre- and post-collision velocities of the particles. Each particle is displaced a distance σ , one in the direction e and the other in the direction $-e$ (see **Figure 1**). Second, the dense hard sphere collision frequency, which contains the so-called Y -factor, is used. With these two simple additions CBA yields the hard sphere equation of state at all densities.

Frezzotti [5] and others [8] have proposed dense gas variants of DSMC based on the Enskog equation [9]. The main advantages of CBA over Enskog-based schemes are its simplicity in implementation and almost negligible effect on computational efficiency for a standard DSMC program. The transport coefficients for CBA, obtained by Green-Kubo analysis, are similar to those of the Enskog equation [1]. As already mentioned, CBA can be extended to potentials other than hard spheres. Besides the standard problems in kinetic theory, CBA has proved useful in the study of granular materials [6] and nuclear physics [7].

Until now the principal deficiency of the Consistent Boltzmann Algorithm was that it lacked a complete theoretical foundation. This paper establishes much of that foundation by deriving the limiting kinetic equation for CBA. This equation is distinct from the Enskog equation and in some respects is easier to manipulate. Besides its relation to CBA, this new equation thus serves as a useful alternative to the Enskog equation in the kinetic theory of dense gases. First, we give a description of the CBA by introducing the corresponding Markov process. Second, we present the limiting (when the number of particles tends to infinity) equation and outline the relationship between this equation and other kinetic equations. Finally, for a toy model, we solve the limiting partial differential equation numerically and illustrate the convergence behaviour of the corresponding stochastic system.

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MARKOV PROCESS

In CBA the interaction of two particles (x, v) and (y, w) is determined by x^* , y^* , v^* , and w^* , the post-collision positions and velocities, respectively. These functions are defined as

$$v^*(x, v, y, w, e) = v + e(e, w - v), \quad w^*(x, v, y, w, e) = w - e(e, w - v)$$

and

$$x^*(x, v, y, w, e) = x + \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|}, \quad y^*(x, v, y, w, e) = y - \sigma \frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|},$$

where $e \in \mathcal{S}^2$, $\mathcal{S}^2 \subset \mathcal{R}^3$ is the unit sphere, and (\cdot, \cdot) , $\|\cdot\|$ denote the scalar product and the Euclidean norm in \mathcal{R}^3 , respectively. If $(e, v - w) = 0$ then define $x^* = x$ and $y^* = y$. The parameter $\sigma \geq 0$ is interpreted as the diameter of the particles. The standard Boltzmann collision transformation is recovered in the case $\sigma = 0$.

The Markov process related to the collision step of the CBA has states of the form $z = \{(x_1, v_1), \dots, (x_n, v_n)\}$ and the infinitesimal generator

$$\mathcal{A}(\Phi)(z) = \frac{1}{2n} \sum_{1 \leq i \neq j \leq n} \int_{\mathcal{S}^2} Q(z, i, j, e) [\Phi(J(z, i, j, e)) - \Phi(z)] de, \quad (1)$$

where the jump transformation is

$$[J(z, i, j, e)]_k = \begin{cases} (x_k, v_k), & \text{if } k \neq i, j, \\ (x^*, v^*), & \text{if } k = i, \\ (y^*, w^*), & \text{if } k = j, \end{cases} \quad (2)$$

and Φ is a bounded measurable test function on the state space. The intensity function has the form

$$Q(z, i, j, e) = Y(\rho) h(x_i, x_j) B(v_i, v_j, e), \quad (3)$$

where h is a mollifying kernel (non-negative approximation of Dirac's delta-function) and B is the Boltzmann collision kernel. The function h depends on the cell structure,

$$h(x, y) = \sum_l \frac{1}{|C_l|} \chi_{C_l}(x) \chi_{C_l}(y), \quad (4)$$

where $|C_l|$ denotes the Lebesgue measure of the cell C_l , and χ is the indicator function. The Enskog Y -factor, $Y(\rho)$, gives the increase in the collision frequency due to ρ , the number density [9] in the given cell, approximated by the state z .

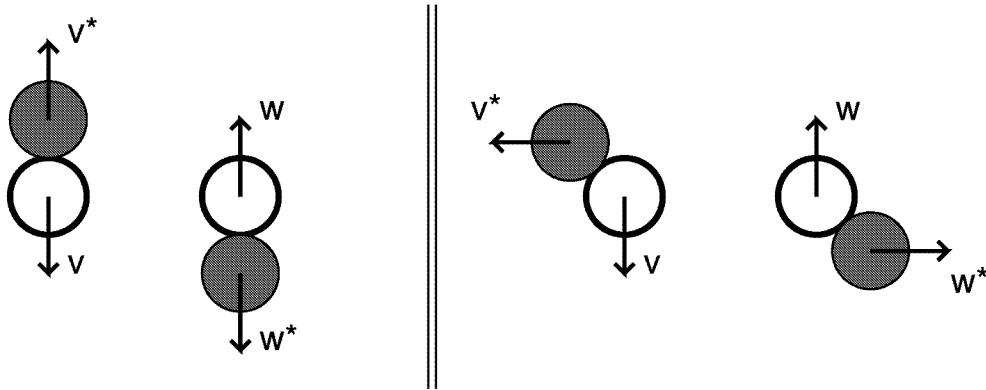


FIGURE 1. Two illustrations of CBA collision displacement for different apse vectors. Before collision the particles have position and velocity (x, v) , (y, w) . After collision the velocities are v^* and w^* ; the shifted positions are indicated by shaded particles.

KINETIC EQUATION

The derivation of the kinetic equation for CBA roughly follows that presented in [11] for DSMC. First one derives the equation satisfied by the limit (as $n \rightarrow \infty$) of the empirical measures of the Markov process. Then the limiting equation for measure-valued functions is transformed into a form for densities. As this derivation is too lengthy to present here, we only give the equation itself,

$$\begin{aligned} \frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x) p(t, x, v) = \\ \int_{\mathcal{R}^3} dw \int_{S^2} de B(v, w, e) \left[Y(\rho(t, x^*)) p(t, x^*, v^*) p(t, x^*, w^*) - Y(\rho(t, x)) p(t, x, v) p(t, x, w) \right], \end{aligned} \quad (5)$$

where p is the probability density. The mollifier (4) is assumed to approach the delta-function, when the number of particles tends to infinity.

Note that in the case $Y \equiv 1$, $\sigma = 0$ the kinetic equation (5) reduces to the **Boltzmann equation**

$$\frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x) p(t, x, v) = \int_{\mathcal{R}^3} dw \int_{S^2} de B(v, w, e) \left[p(t, x, v^*) p(t, x, w^*) - p(t, x, v) p(t, x, w) \right].$$

With $\mathcal{S}_+^2 = \{e : (e, w - v) > 0\}$, equation (5) takes the form

$$\begin{aligned} \frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x) p(t, x, v) = 2 \int_{\mathcal{R}^3} dw \int_{\mathcal{S}_+^2} de B(v, w, e) \times \\ \left[Y(\rho(t, x + \sigma e)) p(t, x + \sigma e, v^*) p(t, x + \sigma e, w^*) - Y(\rho(t, x)) p(t, x, v) p(t, x, w) \right]. \end{aligned} \quad (6)$$

Equation (6) may be contrasted with the **Enskog equation** (cf. [4, Ch.16])

$$\begin{aligned} \frac{\partial}{\partial t} p(t, x, v) + (v, \nabla_x) p(t, x, v) = 2 \int_{\mathcal{R}^3} dw \int_{\mathcal{S}_+^2} de B(v, w, e) \times \\ \left[Y(\rho(t, x + \frac{1}{2} \sigma e)) p(t, x, v^*) p(t, x + \sigma e, w^*) - Y(\rho(t, x - \frac{1}{2} \sigma e)) p(t, x, v) p(t, x - \sigma e, w) \right]. \end{aligned} \quad (7)$$

The **revised Enskog equation** [10] is the same as (7) with the Y -factor replaced with the local-equilibrium pair distribution function.

A TOY MODEL

Here we study an extremely simplified model. For this model the limiting partial differential equation is solved numerically, which allows us to illustrate the convergence behaviour of the stochastic system.

Consider a system where the particles do not have velocities but change their positions during an interaction. The evolution of the system is determined by the generator

$$\mathcal{A}(\Phi)(x) = \frac{B}{2n} \sum_{1 \leq i \neq j \leq n} \int_{S^2} h(x_i, x_j) \left[\Phi(J(x, i, j, e)) - \Phi(x) \right] de, \quad (8)$$

where $x = (x_1, \dots, x_n) \in (\mathcal{R}^3)^n$ and

$$[J(x, i, j, e)]_k = \begin{cases} x_k & , \text{ if } k \neq i, j, \\ x_i + \sigma e & , \text{ if } k = i, \\ x_j - \sigma e & , \text{ if } k = j. \end{cases} \quad (9)$$

Compared with (1)–(3), the function B is a constant, since particle velocities are absent. For simplicity we take $Y = 1$. The analogue of the kinetic equation (5) for this toy model is equation

$$\frac{\partial}{\partial t} p(t, x) = B \int_{S^2} \left[p(t, x + \sigma e)^2 - p(t, x)^2 \right] de. \quad (10)$$

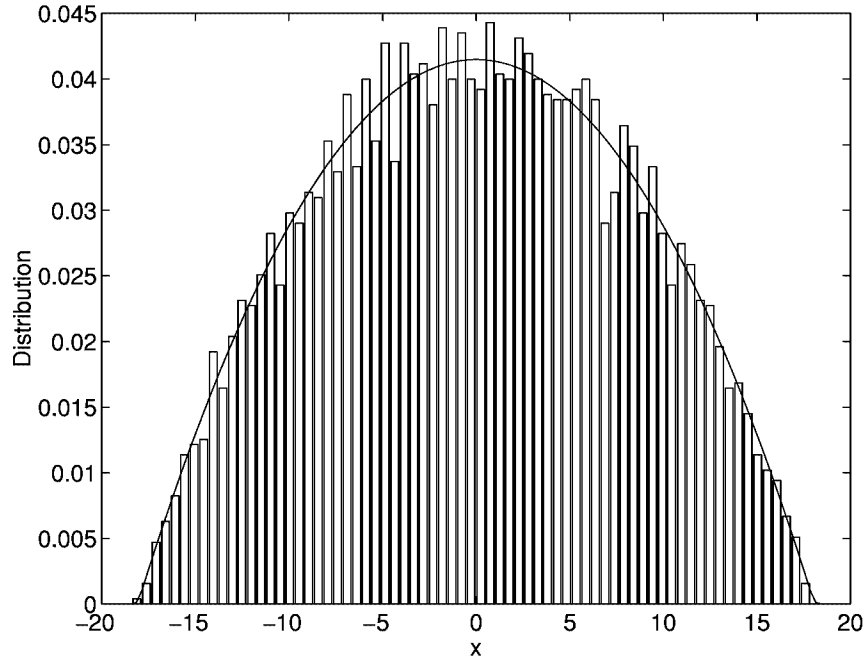


FIGURE 2. Particle distribution in the stochastic system (histogram bars) and probability distribution from the explicit difference scheme (solid line) after 2^{15} time steps.

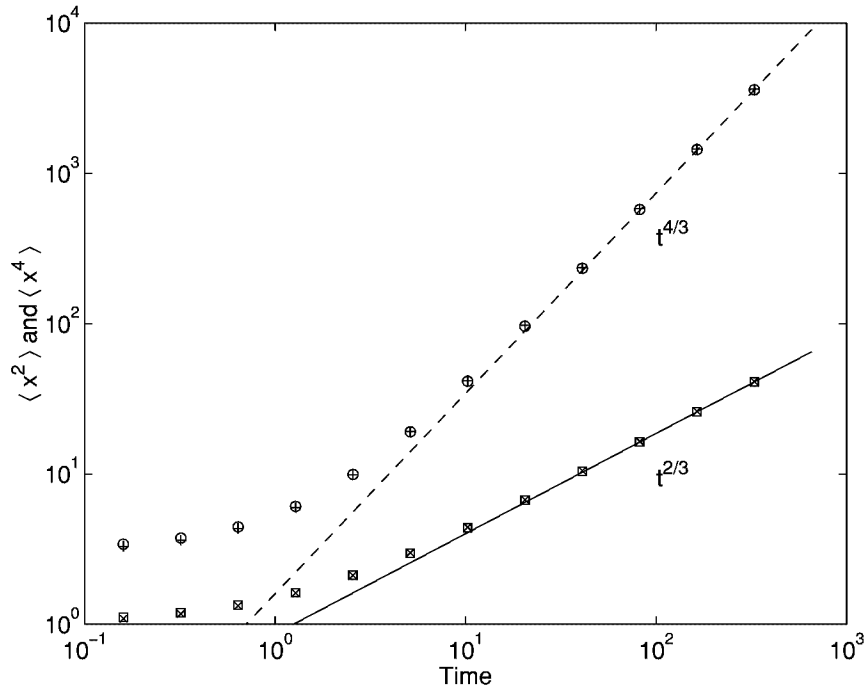


FIGURE 3. Second and fourth moments versus time as measured in the stochastic system (\square and \circ) and in the explicit difference scheme (\times and $+$). The solid and dashed lines go as $t^{2/3}$ and $t^{4/3}$, respectively.

In the one-dimensional case equation (10) takes the form

$$\frac{\partial}{\partial t} p(t, x) = B \left[p(t, x + \sigma)^2 + p(t, x - \sigma)^2 - 2p(t, x)^2 \right]. \quad (11)$$

Note that the unit sphere degenerates to the set $\{-1; 1\}$, where each point is given unit weight. With the choice

$$B = \frac{D}{\sigma^2}, \quad \text{for some constant } D > 0,$$

equation (11) gives in the limit $\sigma \rightarrow 0$ the partial differential equation

$$\frac{\partial}{\partial t} p(t, x) = D \frac{\partial^2}{\partial x^2} p(t, x)^2. \quad (12)$$

An alternative way of writing (12) is

$$\frac{\partial}{\partial t} p(t, x) = \frac{\partial}{\partial x} \mathcal{D} \frac{\partial}{\partial x} p(t, x),$$

where $\mathcal{D} = 2D p(x, t)$ can be viewed as a nonlinear diffusion coefficient.

The results from numerical simulations of the stochastic system (8), (9) and of the explicit difference scheme for equation (11),

$$p(t + \Delta t, x) = p(t, x) + \Delta t D \frac{p(t, x + \sigma)^2 + p(t, x - \sigma)^2 - 2p(t, x)^2}{\sigma^2},$$

are shown in Figures 2 and 3. The stochastic system has 5000 particles. For both the stochastic system and the difference scheme we take $\sigma = 0.3$, $D = 1$, and $\Delta t = 10^{-2}$. The initial distribution is a Gaussian with zero mean and unit variance. The distribution after a long time is bullet-shaped, as shown in **Figure 2**. The second and fourth moments go as $t^{2/3}$ and $t^{4/3}$, as shown in **Figure 3**. These results may be obtained from (12) using scaling arguments. Note that the distribution spreads more slowly than in the standard random walk model for which these moments go as t and t^2 .

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REFERENCES

1. F. J. Alexander, A. L. Garcia, and B. J. Alder. A consistent Boltzmann algorithm. *Phys. Rev. Lett.*, 74(26):5212–5215, 1995.
2. F. J. Alexander, A. L. Garcia, and B. J. Alder. The consistent Boltzmann algorithm for the van der Waals equation of state. *Phys. A*, 240:196–201, 1997.
3. G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon Press, Oxford, 1994.
4. S. Chapman and T. G. Cowling. *The mathematical theory of non-uniform gases. An account of the kinetic theory of viscosity, thermal conduction and diffusion in gases*. Cambridge University Press, London, 1970.
5. A. Frezzotti. A particle scheme for the numerical solution of the Enskog equation. *Phys. Fluids*, 9(5):1329–1335, 1997.
6. H. J. Herrmann and S. Luding. Modeling granular media on the computer. *Contin. Mech. Thermodyn.*, 10(4):189–231, 1998.
7. G. Kortemeyer, F. Daffin, and W. Bauer. Nuclear flow in consistent Boltzmann algorithm models. *Phys. Lett. B*, 374:25–30, 1996.
8. J. M. Montanero and A. Santos. Simulation of the Enskog equation *à la* Bird. *Phys. Fluids*, 9:2057–2060, 1997.
9. P. Resibois and M. De Leener. *Classical Kinetic Theory of Fluids*. Wiley, New York, 1977.
10. H. van Beijeren and M. H. Ernst. The modified Enskog equation. *Physica*, 68:437–456, 1973.
11. W. Wagner. A convergence proof for Bird’s direct simulation Monte Carlo method for the Boltzmann equation. *J. Statist. Phys.*, 66(3/4):1011–1044, 1992.